

# EMERGENT CHIRAL SYMMETRY: PARITY AND TIME REVERSAL DOUBLES

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## Abstract

There are numerous examples of approximately degenerate states of opposite parity in molecular physics. Theory indicates that these doubles can occur in molecules that are reflection-asymmetric. Such parity doubles occur in nuclear physics as well, among nuclei with odd  $A \sim 219-229$ . We have also suggested elsewhere that such doubles occur in particle physics for baryons made up of  $cbu$  and  $cbd$  quarks.

In this article, we discuss the theoretical foundations of these doubles in detail, demonstrating their emergence as a surprisingly subtle consequence of the Born-Oppenheimer approximation, and emphasizing their bundle-theoretic and topological underpinnings. Starting with certain “low energy” effective theories in which classical symmetries like parity and time reversal are anomalously broken on quantization, we show how these symmetries can be restored by judicious inclusion of “high-energy” degrees of freedom. This mechanism of restoring the symmetry naturally leads to the aforementioned doublet structure. A novel by-product of this mechanism is the emergence of an approximate symmetry (corresponding to the approximate degeneracy of the doubles) at low energies which is not evident in the full Hamiltonian. We also discuss the implications of this mechanism for Skyrmin physics, monopoles, anomalies and quantum gravity.

## I. INTRODUCTION

### A. The Born-Oppenheimer Approximation

The degrees of freedom in many systems of physical interest naturally separate into distinct groups organized by their time scales. When this happens, efficient methods of cal-

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culatation can also be frequently devised based on the idea that the time dependence of the slow variables can be ignored in the leading approximation while treating the dynamics of the fast variables.

Molecular physics has many examples with such a sharp differentiation among degrees of freedom [1–3]. Thus the nuclear motion in molecules is a good deal slower than electronic motion, and the former can be treated as slow and the latter as fast. The Born-Oppenheimer (B-O) approximation [2,3] takes advantage of this circumstance by imagining the nuclei to be static when solving for the electronic energy levels. An effective nuclear Hamiltonian  $\hat{\mathcal{H}}_S$  ( $S$  for slow) is then got from the expectation value of the exact Hamiltonian  $\mathcal{H}_S$  in the electronic state, the leading approximation to energy being the eigenvalue of  $\hat{\mathcal{H}}_S$ .

Similar examples can be found in collective nuclear models as well [4–7]. Thus there exist nuclei with slow-moving cores and single-particle excitations over these cores, time scales for the latter being shorter than those for the former. So here too, approximations like that of Born and Oppenheimer can be a satisfactory leading representation of reality.

A third context, of particular interest to particle physicists, concerns bound states of heavy and light quarks [8]. The ratio of  $b$  to  $u$  quark mass is without doubt large while even the  $c$  to  $d$  mass ratio is not negligible by the standards of high energy theory. For example, the value of  $N_c$  in the  $1/N_c$  expansion is 3 whereas the above ratio for constituent masses is approximately 3 to 5. Now we can be confident that quarkonia with several heavy and light quarks will eventually be found, at least when these quarks have long enough lifetimes. It is reasonable to expect that these bound states will share features with molecules and nuclei mentioned above because of the time scales separating heavy and light quarks. That being so, it is plausible to imagine that a Born-Oppenheimer approximation or a variant thereof would be a useful first description of these systems.

## B. Quantum Theory of Shapes

The low-energy bands in molecular physics and collective nuclear models are associated with the rotation of the nucleus as a rigid body. That is to say, we imagine that the configuration space  $Q$  of the nucleus is got by applying rotations to a standard shape  $S_0$  with its center-of-mass at the origin,  $S_0$  being a rigid body with a fixed fiducial orientation relative to a space-fixed reference frame. For methane ( $C_2H_4$ ) with its standard bonds for example,  $S_0$  can be defined as the nucleus with its center-of-mass at the origin, carbon atoms on the third axis and the hydrogen atoms in the 2-3 plane.  $Q$  is the orbit of  $S_0$  under  $SO(3)$  and so is the coset space  $SO(3)/H$ ,  $H$  being the stability group of  $S_0$ . The molecular physicist calls  $H$  the “symmetry group” of  $S_0$ . It follows that the quantum mechanics of nuclei treated as rigid bodies is the quantum mechanics on configuration spaces  $Q = SO(3)/H = SU(2)/H^*$ ,  $H^*$  being the double cover of  $H$ . By systematically specifying all subgroups  $H^*$  of  $SU(2)$ , and all qualitatively distinct quantum theories on  $SU(2)/H^*$ , we can also understand the nature of possible nuclear energy eigenstates and examine their properties.

It is convenient henceforth to think of the double cover  $H^*$  as the ‘symmetry or stability group’ of the rigid body, such as the nucleus being considered. It was denoted by  $H$  in [8].

In previous work [9], we studied quantizations of shapes which we shall understand to be rigid bodies with configuration spaces  $Q = SU(2)/H^*$ . They are topologically non-trivial

and admit several of the striking features we nowadays frequently encounter in quantum field theory. For example, even though functions on  $Q$  are tensorial fields and do not flip sign under  $2\pi$  rotation, there is still the possibility of quantization with spinorial wave functions, a feature reminiscent of Skyrmin physics [10]. For many molecules,  $H^*$  is discrete, and in these cases,  $\pi_1(Q) = H^*$ . In [9], we concentrated on just such molecules and their quantum physics. It is then well-known [10,11] that there is a distinct quantum theory for each unitary irreducible representation (UIR) of  $\pi_1(Q)$ . Wave functions in the domain of the Hamiltonian [12] in one such theory are obtained from smooth sections of the vector bundle associated with its UIR. These theories very nicely show the rich topological and physical effects of twisted bundles with flat connections in perfectly realistic and long familiar systems.

### C. On Quantum Shapes Violating $\mathcal{P}$ and $\mathcal{T}$

In [9], we focussed attention on the effects of  $\pi_1(Q)$  on parity  $\mathcal{P}$  and time reversal  $\mathcal{T}$ . It was found that quantum theories of shapes can violate  $\mathcal{P}$  and  $\mathcal{T}$ . The mechanism is much the same as the one leading to  $\mathcal{P}$  and  $\mathcal{T}$  violation in QCD in the presence of the theta term (for  $\theta \neq 0, \pi$ ):  $\mathcal{P}$  and  $\mathcal{T}$  change the UIR of  $H^*$  to its complex conjugate. In QCD, the analogous result is that  $\mathcal{P}$  and  $\mathcal{T}$  change the UIR  $n \rightarrow e^{in\theta}$  of  $\mathbf{Z}$  to its complex conjugate,  $\mathbf{Z}$  being the fundamental group of the gluon field configuration space.

It merits emphasis that  $\mathcal{P}$  and  $\mathcal{T}$  violation being discussed here is quantum mechanical. The left-right distinction found here is not the same as the distinction between isomeric nuclei. It cannot be seen by a classical physicist. In a similar way, the QCD  $\theta$  has no classical consequence and affects only quantum theory.

In molecular physics, there is no known microscopic source of  $\mathcal{P}$  or  $\mathcal{T}$  violation. For this reason, in ref [9], it was speculated that in a more exact treatment, there must exist mechanisms mixing states mapped to each other by  $\mathcal{P}$  and  $\mathcal{T}$ .

### D. And on How Broken Symmetries are Mended: $\mathcal{P}, \mathcal{T}$ Doubles and Emergent Chiral Symmetry

In this paper, we establish that  $\mathcal{P}$  and  $\mathcal{T}$  are restored in a better treatment in a remarkable and interesting manner. Actually  $\mathcal{P}$  and  $\mathcal{T}$  violation can also happen for rigid bodies with non-discrete  $H^*$ . There are distinct quantum theories associated with distinct UIR's of  $H^*$  here too. As our treatment works equally well for any sort of  $H^*$ , we will present the arguments without requiring its discreteness. It must be mentioned that the work on non-discrete  $H^*$  with emphasis on topology was initiated before by Anezeris, Gupta and Stern [13] and that we will gratefully use their results.

The mathematical account of the mechanism restoring  $\mathcal{P}$  and  $\mathcal{T}$  in molecular and nuclear physics is as follows. Let us assume that the domain  $V^{(\rho_0)}$  of the total Hamiltonian  $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_F$  is associated with the trivial representation  $\rho_0$  and harms neither  $\mathcal{P}$  nor  $\mathcal{T}$ .  $\mathcal{H}_F$  here is the Hamiltonian of the fast variables  $F$  (or the 'fast' Hamiltonian) and  $\mathcal{H}_S$  the Hamiltonian of the slow variables  $S$  (or the 'slow' Hamiltonian). An eigenstate  $\psi_F^{(\overline{\rho})}$  of  $\mathcal{H}_F$  is a section of a vector bundle over  $Q$  in the B-O approximation (the superscripts on the wave

functions indicate the UIR) and it can happen that this bundle is twisted and is associated with a UIR  $\bar{\rho}$ . Standard results on Berry phase [14] demonstrate this possibility. The B-O slow Hamiltonian is not  $\mathcal{H}_S$ , it must be obtained by averaging  $\mathcal{H}$  over  $\psi_F^{(\bar{\rho})}$ , and when that is done, the emergent slow Hamiltonian  $\hat{\mathcal{H}}_S$  contains a connection and has a domain associated with the UIR  $\rho$ , the complex conjugate of  $\bar{\rho}$ . So an eigenstate  $\psi_S^{(\rho)}$  of  $\hat{\mathcal{H}}_S$  corresponds to  $\rho$  and the product wave function  $\psi = \psi_S^{(\rho)} \psi_F^{(\bar{\rho})}$  corresponds to  $\rho \otimes \bar{\rho}$ . But  $\mathcal{H}$  and  $\mathcal{H}_S$  act on the total wave function and their domain can only correspond to  $\rho_0$ . That is now easily arranged as  $\rho_0$  occurs in the reduction of  $\rho \otimes \bar{\rho}$ . The correct total wave function in the B-O approximation is thus the projection  $\chi^{(\rho_0)} = \mathbf{P}[\psi_S^{(\rho)} \psi_F^{(\bar{\rho})}]$  of  $\psi$  to  $V^{(\rho_0)}$ . If the parity transform  $\rho_{\mathcal{P}}$  of  $\rho$  is  $\bar{\rho}$  and hence that of  $\bar{\rho}$  is  $\rho$ , the parity transform  $\mathcal{P}\chi^{(\rho_0)}$  of  $\chi^{(\rho_0)}$  is of the form  $\mathbf{P}[\psi_S^{(\bar{\rho})} \psi_F^{(\rho)}] \in V^{(\rho_0)}$ . It is still in the domain of  $\mathcal{H}$  and  $\mathcal{H}_S$ , so there is no question of  $\mathcal{P}$ -violation. The same goes for  $\mathcal{T}$ . But there is a doubling of states. The doubles with definite  $\mathcal{P}$ , for example, in the leading approximation are linear combinations of  $\chi^{(\rho_0)}$  and  $\mathcal{P}\chi^{(\rho_0)}$ .

In this manner, we can see that when shapes violate  $\mathcal{P}$  or  $\mathcal{T}$ , then we may have  $\mathcal{P}$  or  $\mathcal{T}$  doubles and no  $\mathcal{P}$  or  $\mathcal{T}$  symmetry breakdown after fast variables are included.

There is a simple and vivid manner to understand the physical mechanism behind these doubles. Thus consider for example a molecule like  $N_2O$  [1]. It is a linear molecule with  $O$  at one end and can be approximated by a unit vector  $\vec{n}$  (parallel to the molecule and with the tail at  $O$ ) when finding the rotational levels. The electronic Hamiltonian  $\mathcal{H}_F$  in the B-O approximation is diagonalized by treating  $\vec{n}$  as fixed. Now the system as a whole is rotationally invariant, so for fixed  $\vec{n}$ ,  $\mathcal{H}_F$  is invariant under rotations about the axis  $\vec{n}$ . If  $\vec{L}_F$  is the fast variable angular momentum, an eigenstate of  $\mathcal{H}_F$  can be associated with a definite value of  $\vec{n} \cdot \vec{L}_F$ . It need not be zero, indeed it will not be so for an odd number of electrons, as then no component of  $\vec{L}_F$  has zero eigenvalue. But  $\vec{n} \cdot \vec{L}_F$  reverses under parity  $\mathcal{P}$ , and  $\mathcal{P}$  is a symmetry of  $\mathcal{H}_F$ , so there is another state with the same energy and opposite value of  $\vec{n} \cdot \vec{L}_F$  when the latter is non-vanishing. When we pass beyond the B-O approximation, the exact Hamiltonian  $\mathcal{H}$  mixes these levels, thus creating mutually split even and odd energy eigenstates.

Now of course there are many shapes in nature, and not just those described by  $\vec{n}$ . What is necessary for  $\mathcal{P}$  doubles is that the shape is reflection-asymmetric and singles out an axis. For example, if the molecule is a pyramid with symmetry  $\mathbf{Z}_{2N} \subset SU(2)$  around an axis  $\vec{n}$  [15], then an eigenstate of  $\mathcal{H}_F$  can be associated with a definite value of  $\exp[(2\pi i \vec{n} \cdot \vec{L}_F)/N]$ . [It defines  $\bar{\rho}$ ]. Helicity is defined only mod  $N$ ,  $\vec{n}$  being an  $N$ -fold axis. Nevertheless, since parity inverts the above exponential [and so maps  $\bar{\rho}$  to  $\rho$ ], there are parity doubles unless  $\exp[(2\pi i \vec{n} \cdot \vec{L}_F)/N] = \pm 1$ , that is, unless  $\bar{\rho} = \rho$ .

Parity doubles are also  $\mathcal{T}$ -doubles. That is because  $\mathcal{T}$  reverses  $\vec{L}_F$  and hence  $\vec{n} \cdot \vec{L}_F$ , just as  $\mathcal{P}$  does.

Staggered confirmations in molecular physics are reflection-invariant. They cannot yield  $\mathcal{P}$ -doubles. They can nevertheless give  $\mathcal{T}$ -doubles both with the same  $\mathcal{P}$  value, as we have discussed elsewhere [9]. Such doubles will occur if  $\bar{\rho} \neq \rho$ .

## E. About What is New, What is Predicted, and What Experiments Confirm

The  $\mathcal{P}$ - and  $\mathcal{T}$ - doubles discussed above are *exactly* degenerate in the leading B-O approximation. This exact degeneracy can only be apparent, as there must be transitions between them in a better calculation splitting their energies and leading, for  $\mathcal{P}$ -doubles, to  $\mathcal{P}$ -even and  $\mathcal{P}$ -odd energy eigenstates. This splitting must be small so long as the B-O approximation is decent. We are thus led to suspect the presence of approximately degenerate  $\mathcal{K}$ -doubles, where  $\mathcal{K}$  is either  $\mathcal{P}$  or  $\mathcal{T}$ .

Such parity [and perhaps also time reversal] doubles exist in molecular physics. The ammonia maser is based on such a double. They occur as well in nuclear physics for odd  $A$  in the range 219-229 [6,7]. Elsewhere [8], we have suggested that doubles of this sort can occur among baryons, Skyrmions and also composites containing grand unified monopoles. We will recall our suggestions in particle physics later on in this work. But our primary concern in this paper is with the bundle-theoretic aspects of these doubles. While the computational basis of these doubles is well-understood by chemists and nuclear physicists, their bundle-theoretic significance is not even mentioned in their traditional literature. It is only in modern times, after growth of interest in Berry's phase, that Moody, Shapere and Wilczek [2] elucidated formal aspects of the B-O approximation. Our work further elaborates on these aspects, with special emphasis on  $\mathcal{P}$ - and  $\mathcal{T}$ - symmetry restoration by the fast variables and the attendant emergence of  $\mathcal{P}$ - and  $\mathcal{T}$ - doubles, and covers also twisted bundles of any rank over the slow variable configuration space. We do not think that  $\mathcal{P}$  and  $\mathcal{T}$  restoration and the doubles emergent therefrom, or the higher rank bundles have been discussed with adequate gravity before.

Summing up, we intend to review known results in current bundle- and domain-theoretic language, extend them in novel directions, emphasize their striking features and connect them to known phenomena in quantum field theory like the QCD  $\theta$ . The new language has power and generality, and adapted for research in original directions. Indeed, using the experience gained from the foregoing considerations with  $SU(2)/H^*$  as the "slow" manifold, we will be able to develop the general bundle-theoretic setting for the B-O approximation when  $Q$  is any manifold and not limited to  $SU(2)/H^*$ . This work will then also be helpful in studying rather new applications of these ideas in Skyrmon physics, quantum gravity and elsewhere. All these matters will be taken up for consideration later on in this paper.

## F. A Speculation about Macroscopic Chirality

In [9], we had speculated on a scenario for the emergence of macroscopic classical left-right asymmetries in nature from the physics of these doubles. At the level of individual doubles, their classical description gives no clue about their difference. Nevertheless, it was suggested that because of quantum effects, their aggregates can lead to macroscopic chirality as follows: it can happen that chiral molecular samples having a dominant admixture of molecules with wave functions  $\psi_S^{(\rho)}\psi_F^{(\bar{\rho})}$  or  $[\psi_S^{(\bar{\rho})}\psi_F^{(\rho)}] \in V^{(\rho_0)}$  are formed in nature. They can get formed, although they are not energy eigenstates, for example by the action of polarized morning sunlight. If their decay time into energy eigenstates is sufficiently large, they can unite and bind into larger chiral molecules among themselves or with other neighbouring

atoms or molecules. These bigger chiral structures would be expected to live longer too because of their size and may very well display macroscopic classical chirality. The latter is stimulated in this proposal by the microscopic quantum mechanical  $\mathcal{P}$ - asymmetry. They may even be stable. In this way, we can conceive of the formation of macroscopic chiral structures like those actually encountered in nature.

The above scenario is speculative, but conceivable. Thus in the ammonia molecule for example, the parity doubles are separated by  $1 \text{ cm}^{-1}$  while the rotational energies are of the order  $20 \text{ cm}^{-1}$ . Their ratio of  $\sim 0.05$  would also be approximately the ratio of the nuclear rotation period to the lifetime of the chiral state, so the latter ratio is large. There are numerous molecular parity doubles with similar large numbers. It is now an interesting matter, open for investigation, to confirm or deny this scenario by detailed calculations.

## G. Contents of the Paper

Quantization of shapes in modern language, and the demonstration that they can violate  $\mathcal{P}$  and  $\mathcal{T}$  by quantum mechanical effects, have been fully covered in [9]. We will briefly summarize the results of that reference in Section 2. In Section 3, we take up the treatment of the fast variables for the “slow” configuration space  $Q = SU(2)/H^*$  and derive the general form of the eigenfunctions  $\psi_F^{(\bar{\rho})}$  of  $\mathcal{H}_F$  as sections of a vector bundle over  $Q$ . The bundle is associated with the UIR  $\bar{\rho}$  of  $H^*$ . The fast variables  $F$  can describe electrons in molecular physics and “intrinsic components” [4] or excitations over the core in nuclear physics. Such details are not important at our level of generality. In Section 4, we derive the effective Hamiltonian  $\hat{\mathcal{H}}_S$  for the above  $Q$ . It now contains a connection induced by the fast variables. The connection determines the bundle appropriate for the slow variables. This bundle is associated with the representation  $\rho$  complex conjugate to  $\bar{\rho}$ . The nature of the total wave function claimed earlier is in this manner established. There is no  $\mathcal{P}$  or  $\mathcal{T}$  violation in the total system even though there could be such violation in the quantum theory of just the shapes if  $\rho \neq \bar{\rho}$ .

Calculations of the sort we perform here for the derivation of  $\hat{\mathcal{H}}_S$  have appeared elsewhere before [16,2].

In Section 5, after recapitulating the nature of the total wave functions and how  $\mathcal{P}$  and  $\mathcal{T}$  are restored as symmetries, we explain a standard mechanism mixing the wave functions  $\psi_S^{(\rho)}\psi_F^{(\bar{\rho})}$  and  $\psi_S^{(\bar{\rho})}\psi_F^{(\rho)}$ . It is this which splits the parity and time reversal doubles in the leading order.

Section 6 discusses the possibility of  $\mathcal{P}$ - and  $\mathcal{T}$ - doubles in quark physics and argues in particular that they may occur in *cbu* or *cbd* systems. The difference between the conventional quark model states and these B-O states is also pointed out. Certain other areas of interest to particle physics where the Born-Oppenheimer ideas may be fruitful are postponed for discussion to Section 8.

Section 7 develops the theory of the B-O approximation when  $Q$  is not just  $SU(2)/H^*$ , but a more general manifold. The concluding Section 8 indicates how Section 7 can be applied to Skyrmion and monopole physics, anomalies and quantum gravity. Work on all these topics is in progress with promising results.

## II. WHEN DO SHAPES VIOLATE $\mathcal{P}$ AND $\mathcal{T}$ ?

The total Hamiltonian  $\mathcal{H}$  of the slow and fast variables can be written as the sum of two terms:

$$\mathcal{H} = \mathcal{H}_S + \mathcal{H}_F. \quad (2.1)$$

In this decomposition,  $\mathcal{H}_S$  depends only on the slow degrees of freedom. Its typical form when  $S$  is a shape with configuration space  $SU(2)/H^*$  is

$$\mathcal{H}_S = \vec{L}_S^2 / 2\mathcal{I}, \quad (2.2)$$

$\vec{L}_S$  being the angular momentum of  $S$  and  $\mathcal{I}$  its moment of inertia. The Hamiltonian  $\mathcal{H}_F$  contains the fast degrees of freedom and also the interaction between  $S$  and  $F$ .

*The discussion in this section concerns  $\mathcal{H}_S$ .* It is important to recognize that  $\mathcal{H}_S$  is not the B-O slow Hamiltonian  $\hat{\mathcal{H}}_S$  emergent from the average of  $\mathcal{H}$  over  $\psi_F^{(\bar{\rho})}$ . The distinction is of particular significance for nonabelian  $\bar{\rho}$ . We will resume further examination of  $\hat{\mathcal{H}}_S$  and  $\mathcal{H}_S$  in later sections.

The symmetry groups  $H^*$  of shapes can be discrete or continuous. Our discussion applies to all choices of  $H^*$ . For a classical shape with configuration space  $Q = SU(2)/H^*$ , there is a quantum shape for each UIR  $\rho$  of  $H^*$  [9–11]. Wave functions in the domain of the Hamiltonian are sections of the vector bundle over  $Q$  associated with the representation  $\rho$ . They can be found as follows [17].

Let  $[\rho]$  be the dimension of the UIR  $\rho$  and  $\rho(h)$  the matrix of  $h \in H^*$  in  $\rho$ . The above wave functions are constructed from smooth vector-valued functions  $f$  on  $SU(2)$  with “internal” dimension  $[\rho]$ ,

$$f = (f_1, f_2, \dots, f_{[\rho]}), \quad f_j(g) \in \mathbf{C} \text{ for } g \in SU(2), \quad (2.3)$$

which also have the transformation property

$$f_j(gh) = f_k(g)\rho_{kj}(h), \quad h \in H^*. \quad (2.4)$$

### A. Discrete $H^*$

When  $H^*$  is discrete, the fibres of the principal bundle  $H^* \rightarrow SU(2) \rightarrow SU(2)/H^*$  are also discrete. In this case, the Hamiltonian  $\mathcal{H}_S$  can be defined as a self-adjoint operator on the wave functions (2.3) for any choice of  $\rho$ . This is because the connection in the above bundle is flat [9–11, 17]. There is thus a certain freedom in the choice of the domain for  $\mathcal{H}_S$  with its attendant quantization ambiguity mentioned above.

Discrete symmetry groups occur for pyramids, tetrahedra, and eclipsed conformations (with dihedral symmetry groups). For these shapes, it was shown in [9] that  $\mathcal{P}$  or  $\mathcal{T}$  violation will occur if and only if  $\rho \neq \bar{\rho}$ . In contrast, staggered conformations (also with dihedral symmetry groups) never violate  $\mathcal{P}$  while they continue to violate  $\mathcal{T}$  if  $\rho \neq \bar{\rho}$ . Hence they can also violate  $\mathcal{PT}$ .

The cube and the dodecahedron, and their duals, the octahedron and icosahedron, also have discrete symmetry groups, but they cannot violate  $\mathcal{P}$  or  $\mathcal{T}$  [9].

### B. The Case $H^* = U(1)$

$SU(2)$  has a  $U(1)$  subgroup which is unique up to conjugation. It can be taken to be

$$U(1) = \{e^{i\tau_3\theta/2} : 0 \leq \theta \leq 4\pi\}, \quad \tau_i = \text{Pauli matrices.} \quad (2.5)$$

The space  $Q = SU(2)/U(1)$  is the two-sphere  $S^2$  of unit vectors or arrows with heads [10]:

$$S^2 = \{\vec{n} : \vec{n} \in \mathbf{R}^3, \vec{n} \cdot \vec{n} = 1\}. \quad (2.6)$$

The stability group of  $\vec{n}$  is  $U(1)$ . The latter is the stability group of any shape with axial symmetry. Any such shape has the above configuration space  $Q$ .

The UIR's  $\rho = \rho_K (K \in \mathbf{Z}/2)$  of  $H^* = U(1)$  are given by

$$\rho_K : e^{i\tau_3\theta/2} \rightarrow \rho_K(e^{i\tau_3\theta/2}) = e^{iK\theta}. \quad (2.7)$$

The functions (2.3) for  $\rho = \rho_K$  give sections of  $U(1)$  bundles over  $S^2$  for Chern class  $K$ . These are the bundles for charge-monopole systems with  $K = eg/4\pi$ ,  $e$  and  $g$  being the electric and magnetic charges [10]. Now just as for the latter,  $\mathcal{P}$  and  $\mathcal{T}$  change  $\rho_K$  to  $\rho_K^*$ , or  $K$  to  $-K$ , and hence are violated for  $K \neq 0$ . But  $\mathcal{PT}$  is always good.

When  $H^* = U(1)$ , the Hamiltonian  $\mathcal{H}_S$  itself completely determines the bundle, that is, the choice of  $K$ . This is because the bundles for  $K \neq 0$  do not admit flat connections. The Hamiltonian  $\mathcal{H}_S$  is not (2.2), but rather has the general form

$$\vec{\mathcal{L}}_S^2/2\mathcal{I}, \quad (2.8)$$

$\vec{\mathcal{L}}_S = \vec{L}_S +$  a term involving the connection appropriate for  $\rho_K$ . For example,  $\vec{\mathcal{L}}_S$  can be  $\vec{r} \times (\vec{p} - e\vec{A})$  where  $\vec{r}$  and  $\vec{p}$  are the relative coordinate and its conjugate momentum,  $\vec{A}$  is the vector potential of the monopole field  $(g/4\pi)\vec{r}/r^3$  and the entire expression is restricted to the two-sphere  $\vec{r} = \vec{n}$ .

### C. The case $H^* = D_\infty^*$

$SU(2)$  has yet another non-discrete subgroup which is also unique up to conjugation. It is the ‘infinite’ dihedral group

$$D_\infty^* = \{e^{i\tau_3\theta/2}, i\tau_2 : 0 \leq \theta \leq 4\pi\}, \quad (2.9)$$

$i\tau_2$  being rotation by  $\pi$  around the second axis. The shape  $Q = SU(2)/D_\infty^*$  is the projective two-sphere of headless arrows:

$$Q = \mathbf{RP}^2, \quad (2.10)$$

the headless arrow having  $D_\infty^*$  (or rather, a group isomorphic to (2.9)) as its stability group. The hydrogen molecule is an example described by a headless arrow and the configuration space  $\mathbf{RP}^2$ .



The one-dimensional UIR's of  $D_\infty^*$  are the trivial one (which need not be discussed further) and the representation

$$\begin{aligned}\rho : e^{i\tau_3\theta/2} &\rightarrow 1, \\ i\tau_2 &\rightarrow -1.\end{aligned}\tag{2.11}$$

It also has the two-dimensional UIR's

$$\rho_K : e^{i\tau_3\theta/2} \rightarrow \rho_K(e^{i\tau_3\theta/2}) = \begin{bmatrix} e^{iK\theta} & 0 \\ 0 & e^{-iK\theta} \end{bmatrix},\tag{2.12}$$

$$i\tau_2 \rightarrow \rho_K(i\tau_2) = i\tau_2,\tag{2.13}$$

$$K \in \mathbf{N}/2.\tag{2.14}$$

The group  $\rho(D_\infty^*)$  is the discrete group  $\mathbf{Z}_2$ . In this case, just as for the discrete  $H^*$ , there is a two-fold ambiguity in quantizing  $\mathcal{H}_S$ : we can use either the trivial UIR or the UIR (2.11).

Let  $|m\rangle$ ,  $m \in \{j, -j+1, \dots, j\}$  be the standard orthonormal basis for the  $(2j+1)$ -dimensional UIR of  $SU(2)$  with the 3rd component  $J_3^{(j)}$  of angular momentum being diagonal:

$$J_3^{(j)}|m\rangle = m|m\rangle,\tag{2.15}$$

$$\langle m'|m\rangle = \delta_{m'm}.\tag{2.16}$$

Choose  $j$  so that  $\pm K$  occur in the spectrum of  $J_3^{(j)}$ . Then the restriction of

$$e^{iJ_3^{(j)}\theta}, \quad e^{iJ_2^{(j)}\pi}$$

to the subspace spanned by  $|K\rangle$  and  $|-K\rangle$  gives the UIR  $\rho_K$ ,  $J_2^{(j)}$  here being the second component of angular momentum.

A headless arrow is invariant under reflection. So we can set  $\mathcal{P} = 1$  on wave functions and there is no parity violation for any of the UIR's of  $\mathbf{RP}^2$ .

There is no  $\mathcal{T}$  violation either for any of the UIR's of  $\mathbf{RP}^2$ . That is because the one-dimensional UIR's are real while the UIR's  $\bar{\rho}_K$  complex conjugate to  $\rho_K$  is equivalent to  $\rho_K$ :

$$\bar{\rho}_K(h) = \rho_K(i\tau_2)\rho_K(h)\rho_K^{-1}(i\tau_2), h \in D_\infty^*.\tag{2.17}$$

The UIR  $\rho_K(D_\infty^*)$  is not discrete. So the option of using this representation is available only if the Hamiltonian itself is of the form (2.8). Now as  $\rho_K$  is two-dimensional, it is a  $2 \times 2$  matrix of differential operators. We will discuss such operators further in Section 4.

### III. THE FAST WAVE FUNCTION

As mentioned in the Introduction, until Section 7, we will specialize to the case  $SU(2)/H^*$  for the slow configuration space  $Q$ . We will also occasionally explain or illustrate a point using molecules as they provide excellent examples for these  $Q$ .

A fast wave function for us means an energy eigenstate for the Hamiltonian  $\mathcal{H}_F$  in the B-O approximation. The slow variables of the shape are looked upon as static in this approximation.

Let us assume that the total Hamiltonian  $\mathcal{H}$  for the interacting fast and slow variables is rotationally invariant. This assumption can be avoided as shown in Section 7, but is realistic, so let us keep it for now.

Let  $S_0$  be the conveniently chosen standard shape. The group  $SU(2)$ , the two-fold cover of  $SO(3)$  of spatial rotations, acts transitively on  $Q$ . Denoting this action by  $S_0 \rightarrow gS_0$ ,  $g \in SU(2)$ , any shape  $S$  can be written as  $gS_0$ .

Let  $H^*$  be the subgroup of  $SU(2)$  leaving  $S_0$  invariant. Then the invariance group of  $gS_0$  is  $gH^*g^{-1}$ . It is isomorphic to  $H^*$ , but not identical to  $H^*$  when regarded as a subgroup of  $SU(2)$ .

The group  $SU(2)$  acts on the operators  $\mathcal{O}_F$  intrinsic to the fast system and on the eigenstates  $|\cdot\rangle$  of  $\mathcal{H}_F$ . Let us denote these actions by  $\mathcal{O}_F \rightarrow U(s)\mathcal{O}_FU(s)^{-1}$  and  $|\cdot\rangle \rightarrow U(s)|\cdot\rangle$ ,  $s \in SU(2)$ ,  $U(s)$  being a unitary operator. Let  $\vec{L}_F$  be the generators of this  $SU(2)$ . They are the fast angular momenta.

As  $\mathcal{H}$  is invariant under  $SU(2)$  and  $hS_0 = S_0$  for  $h \in H^*$ ,  $\mathcal{H}_F$  is invariant under the  $H^*$  action on  $F$  alone when the slow variable has the configuration  $S_0$ . Eigenfunctions of  $\mathcal{H}_F$  for a fixed eigenvalue will therefore transform by a representation of  $H^*$ . This representation will be UIR unless there is “accidental” degeneracy as for the non-relativistic hydrogen atom. Results for a general representation, which will be a direct sum of UIR’s, in any case follow from those for the latter, so let us assume the representation to be a UIR  $\bar{\rho}$ .

Suppose then that the shape is  $S_0$  and that for that shape,

$$\{|m\rangle = m \in \text{a suitable index set } \bar{I}\} \quad (3.1)$$

is an orthonormal basis spanning an eigenstate of  $\mathcal{H}_F$  and carrying also the UIR  $\bar{\rho}$ :

$$\begin{aligned} \mathcal{H}_F|m\rangle &= \epsilon|m\rangle, \\ U(h)|m\rangle &= |m'\rangle\bar{\rho}(h)_{m'm}, \\ \langle m'|m\rangle &= \delta_{m'm}. \end{aligned} \quad (3.2)$$

The corresponding states when the shape is  $gS_0$  are just  $U(g)|m\rangle$ :

$$\begin{aligned} \mathcal{H}_FU(g)|m\rangle &= \epsilon U(g)|m\rangle, \\ \langle m'|U(g)^\dagger U(g)|m\rangle &= \delta_{m'm}. \end{aligned} \quad (3.3)$$

As shown here, the new states are orthogonal since  $U(g)$  is unitary. [The background shape in  $\mathcal{H}_F$  here is  $gS_0$  while it is  $S_0$  in (3.3). Still, for notational simplicity, we have denoted this operator by the same symbol  $\mathcal{H}_F$  used in (3.3) although this is not quite correct.]

The eigenvalue  $\epsilon$  has no shape dependence because of the assumed  $SU(2)$  invariance of  $\mathcal{H}_F$ .

A fast wave function depends not only on  $g$  and  $m$ , but also on variables  $\{\xi_\beta\}$  describing the fast configuration in the body-fixed frame of the slow variables. They are invariant under  $SU(2)$ , being the analogues of radial coordinates for a particle in a central potential. It is

convenient to rewrite  $|m\rangle$  in a particular way where this and angular momentum dependence can be made explicit.

So let us expand  $|m\rangle$  in a basis  $|m, j\rangle$  where  $\vec{L}_F^2$  is diagonal:

$$\begin{aligned}\vec{L}_F^2|m, j\rangle &= j(j+1)|m, j\rangle, \\ \langle m', j'|m, j\rangle &= \delta_{m'm}\delta_{j'j}.\end{aligned}\tag{3.4}$$

The expansion is

$$\begin{aligned}|m\rangle &= \sum_j |m, j\rangle \alpha_j, \\ \alpha_j : \{\xi_\beta\} &\rightarrow \alpha_j(\{\xi_\beta\}) \in \mathbf{C}.\end{aligned}\tag{3.5}$$

Of course a  $j$  would occur in the sum here only if the spin  $j$  UIR of  $SU(2)$  on restriction to  $H^*$  contains  $\bar{\rho}$ .

Let  $d\mu(\{\xi_\beta\})$  be the measure of integration for the scalar product of functions of  $\{\xi_\beta\}$ . Then the orthonormality of  $|m\rangle$  gives

$$\int d\mu(\{\xi_\beta\}) \sum_j |\alpha_j(\{\xi_\beta\})|^2 = 1.\tag{3.6}$$

We can expand  $\alpha_j$  in a complete set of functions orthonormal for the measure  $d\mu(\{\xi_\beta\})$  if desired.

A basis  $\{|k, j\rangle\}$  of  $(2j+1)$  orthonormal states spanning the spin  $j$  UIR of  $SU(2)$  can be chosen so that  $\{|m, j\rangle : m \in \bar{I}\} \subset \{|k, j\rangle\}$ :

$$\begin{aligned}\langle k', j'|k, j\rangle &= \delta_{k'k}\delta_{j'j}, \\ \{|m, j\rangle : m \in \bar{I}\} &\subset \{|k, j\rangle\}.\end{aligned}\tag{3.7}$$

In this basis,

$$U(s)|m, j\rangle = |k, j\rangle D_{km}^j(s), m \in \bar{I}\tag{3.8}$$

where  $k$  is summed over  $(2j+1)$  values and  $D^j(s)$  are the rotation matrices in the chosen basis. Thus we get the useful formula

$$\chi_m^F(g, \cdot) \equiv U(g)|m\rangle = \sum |k, j\rangle D_{km}^j(g) \alpha_j(\cdot).\tag{3.9}$$

A property of significance is the following transformation of  $\chi_m^F$  implied by (3.9):

$$\chi_m^F(gh, \cdot) = \chi_{m'}^F(g, \cdot) \bar{\rho}(h)_{m'm}.\tag{3.10}$$

#### IV. THE SLOW WAVE FUNCTION

The effective “slow” Hamiltonian  $\hat{\mathcal{H}}_S$  for the slow degrees of freedom in the B-O approximation differs in general from the “true” slow Hamiltonian  $\mathcal{H}_S$ . An energy eigenstate of  $\hat{\mathcal{H}}_S$ ,

or perhaps of  $\mathcal{H}_S$ , is what we informally and indiscriminately call the slow wave function. It thus refers to a wave function with dependence only on slow variables.

The slow variables belong to massive bodies. Their spin effects, which depend on powers of inverse mass, are therefore small and are ignored in the B-O approximation.

In molecular physics, while discussing rotational bands in the B-O approximation, all degrees of freedom of the nucleus except its overall shape are frozen. The nature of the angular momentum for the slow system is thus of central importance in this approximation. We will make the following assumption about it in what follows: for the Hamiltonians  $\mathcal{H}_S$  and  $\mathcal{H}$ , and hence for the exact slow wave functions, it is just the orbital angular momentum  $\vec{L}_S$ .

While discussing  $\vec{L}_S$ , we can put the center-of-mass of the slow system at the origin, and when talking about molecules distribute the constituent nuclei so that altogether they have the symmetry group  $H^*$ . We can for example imagine them to be connected by chemical bonds. Then components of  $\vec{L}_S$  become just the vector fields generating rotations. Their domain of definition being obtained from smooth functions on  $Q$ , and with  $\mathcal{H}_S$  being (2.2), the bundle of slow wave functions on  $Q$  is trivial. This then is the content of our assumption whether or not we are dealing with molecular physics.

We restrict angular momentum in this manner partly for convenience. It could happen for a general system that the angular momentum of the (exact) slow system is not  $\vec{L}_S$ , but a twisted version thereof appropriate for some nontrivial bundle over  $Q$ . But this case can be dealt with effortlessly with minor modifications of our discussion. As for molecular physics, when the effects of spin  $\vec{S}$  of the slow constituents are not ignored, the angular momentum is not  $\vec{L}_S$ , but  $\vec{J} = \vec{L}_S + \vec{S}$ ,  $\vec{S}$  being the total spin. If the time scales associated with the motion of spins are short, we can treat  $\vec{S}$  too as a fast variable. It could then acquire a non-zero component along the body-fixed axis. The form of angular momentum would then be altered and the bundle of slow wave functions over  $Q$  would get twisted. In that event we must modify the discussion somewhat, but the changes are cosmetic, as we can include  $\vec{S}$  too among fast variables. No separate discussion is thus needed when the effects of spin of the slow system are not ignored provided spin is fast. But that is not the case if  $\vec{S}$  for example is not fast. This situation will not be covered in this paper.

The eigenstate of  $\mathcal{H}$  in the B-O approximation is assumed to have the form

$$\phi = \sum \psi_S^m \chi_m^F \quad (4.1)$$

where  $\psi_S^m$  is a function only of the slow variables. [Here  $\chi_m^F$  depends on  $g$  and  $\{\xi_\beta\}$ ,  $\chi_m^F(g, \cdot)$  being the function of  $\{\xi_\beta\}$  in (3.9)]. Hence

$$\mathcal{H}\phi = \mathcal{H}_S \sum \psi_S^m \chi_m^F + \epsilon \sum \psi_S^m \chi_m^F. \quad (4.2)$$

We now average this over the fast degrees of freedom. On taking the scalar product with  $\chi_m^F$ , the eigenvalue problem

$$\mathcal{H}\phi = E\phi \quad (4.3)$$

becomes

$$\sum_n (\chi_m^F, \mathcal{H}_S \chi_n^F) \psi_S^n + \epsilon \psi_S^m = E \psi_S^m \quad (4.4)$$

In the traditional B-O approximation, only the intermediate states  $\chi_j^F$  are retained between the two  $\vec{L}_S$  when evaluating the first term using (2.2). In this approximation, this kinetic energy term  $\vec{L}_S^2/2\mathcal{I}$  becomes  $\vec{\mathcal{L}}_S^2/2\mathcal{I}$ , where  $\mathcal{L}_{Sj}$  are matrix-valued differential operators:

$$(\vec{\mathcal{L}}_S)_{mn} = \delta_{mn}\vec{L}_S + (\chi_m^F, [\vec{L}_S \chi_n^F]). \quad (4.5)$$

The square brackets here signify that  $\vec{L}_S$  within it differentiates only  $\chi_n^F$  ( and not objects which may occur further to the right).

There is a certain delicacy in the definition of  $\vec{\mathcal{L}}_S$  in (4.5) since orbital angular momentum acts on functions on  $Q$  whereas  $\psi_S^m$  and  $\chi_n^F$  depend on  $g$ . We will address this issue later on in Section 5.

The B-O slow Hamiltonian and the equation for energy are therefore [3,2,16]

$$\begin{aligned} \hat{\mathcal{H}}_S &= \vec{\mathcal{L}}_S^2/2\mathcal{I} + \epsilon, \\ \hat{\mathcal{H}}_S \psi_S &= E \psi_S, \quad \psi_S = (\psi_S^1, \psi_S^2, \dots). \end{aligned} \quad (4.6)$$

The operator  $\vec{\mathcal{L}}_S$  is not always an angular momentum. Its components need not fulfill angular momentum commutation relations. But we want to know the angular momentum commuting with  $\hat{\mathcal{H}}_S$ , or rather, the bundle describing the energy levels of  $\hat{\mathcal{H}}_S$ . We can address this task as follows.

The choice of  $|m\rangle$  is not unique. We can get another choice by the action of an  $h$  in  $H^*$ . Thus we can change  $|m\rangle$  to  $|m'\rangle \bar{\rho}(h)_{m'm}$  and thereby also change  $\chi_m^F$  according to

$$\chi_m^F \rightarrow \chi_{m'}^F \bar{\rho}(h)_{m'm}. \quad (4.7)$$

This corresponds just to the change

$$\chi_m^F(g, \cdot) \rightarrow \chi_m^F(gh, \cdot) \quad (4.8)$$

in the choice of basis for energy eigenfunctions of  $\hat{\mathcal{H}}_S$ .

The responses of  $\vec{\mathcal{L}}_S$  and  $\hat{\mathcal{H}}_S$  to the transformation (3.10) are

$$\begin{aligned} \vec{\mathcal{L}}_S &\rightarrow \bar{\rho}(h)^{-1} \vec{\mathcal{L}}_S \bar{\rho}(h), \\ \hat{\mathcal{H}}_S &\rightarrow \bar{\rho}(h)^{-1} \hat{\mathcal{H}}_S \bar{\rho}(h). \end{aligned} \quad (4.9)$$

The response of  $\psi_S$  is thus

$$\psi_S \rightarrow \bar{\rho}(h)^{-1} \psi_S. \quad (4.10)$$

The group  $SU(2)$  as a manifold is an  $H^*$ -principal bundle over  $Q = SU(2)/H^*$ . It is convenient to regard  $\psi_S$  as a function on  $SU(2)$ . [The conventional wave function, which is a section of an associated bundle can be obtained by a “gauge choice”, that is by restricting the above  $\psi_S$  to a section of this principal bundle.] It thus follows that

$$\psi_S(gh) = \bar{\rho}(h)^{-1} \psi_S(g). \quad (4.11)$$

As  $\bar{\rho}$  is unitary, we thus get

$$\psi_S^m(gh) = \psi_S^{m'}(g) \rho(h)_{m'm} \quad (4.12)$$

where  $\rho$  is the UIR complex conjugate to  $\bar{\rho}$ . So  $\psi_S$  comes from the associated vector bundle for the UIR complex conjugate to the UIR of the fast wave function [2].

The  $SU(2)$  group of angular momentum acts on  $\psi_S$  by left multiplication on  $g$ . If  $U(g')$  is the corresponding unitary operator, this action explicitly is

$$[U(g')\psi_S](g) = \psi_S(g'^{-1}g). \quad (4.13)$$

The expression for angular momentum can be written down from the infinitesimal form of this formula.

Note that as  $g'$  acts on the left, and  $h$  on the right, of  $g$ , these two actions commute.

### A. Emergence of Unitary Gauge Symmetries

In the above discussion, we limited ourselves to transformations of  $\chi_m^F$  induced by  $H^*$ . There is no good reason for this restraint, we can transform them by any unitary transformation and they will still remain orthonormal and degenerate eigenstates of  $\mathcal{H}_F$ . We can even choose the elements of the unitary matrix to be functions on  $Q$  without spoiling these properties. Thus the general transformation we can perform is

$$\chi_m^F(g, \cdot) \rightarrow \chi_{m'}^F(g, \cdot) u_{m'm}(g S_o) \quad (4.14)$$

where we have labeled points of  $Q$  by the shapes  $g S_o$ . These transformations form the unitary gauge group  $u_{[\bar{\rho}]}$ ,  $[\bar{\rho}]$  being the dimension of the UIR  $\bar{\rho}$ .

Let  $\vec{A}$  be the  $[\bar{\rho}] \times [\bar{\rho}]$  matrix with components

$$\vec{A}_{mn} = (\chi_m^F, [\vec{L}_S \chi_n^F]). \quad (4.15)$$

Its response to the transformation (4.14) is

$$\vec{A} \rightarrow u^{-1} \vec{A} u + u^{-1} [\vec{L}_S u]. \quad (4.16)$$

This shows that  $\vec{A}$  is a connection for the above gauge group.

The transformation properties of  $\vec{\mathcal{L}}_S$ ,  $\hat{\mathcal{H}}_S$  and  $\psi_S$  are

$$\vec{\mathcal{L}}_S \rightarrow u^{-1} \vec{\mathcal{L}}_S u, \quad (4.17)$$

$$\hat{\mathcal{H}}_S \rightarrow u^{-1} \hat{\mathcal{H}}_S u, \quad (4.18)$$

$$\psi_S^m \rightarrow \psi_S^{m'} u_{m'm}^*. \quad (4.19)$$

Thus a unitary gauge group has emerged from the B-O approximation.

The functions  $u_{m'm}$  on  $Q$  can be thought of as functions  $\hat{u}_{m'm}$  on  $SU(2)$ :

$$u_{m'm}(g S_0) = \hat{u}_{m'm}(g). \quad (4.20)$$

They are not general functions on  $SU(2)$  however, having the invariance property

$$\hat{u}_{m'm}(gh) = \hat{u}_{m'm}(g) \quad \text{for } h \in H^*. \quad (4.21)$$

It is natural to enquire if the gauge group can be further enlarged by dropping this restriction. The resultant gauge transformations  $\{\hat{v}\}$  would consist of functions on  $SU(2)$  with values in  $[\bar{\rho}]$ - dimensional unitary matrices. They would not be constrained by an equation like (4.21). So they cannot always be regarded as functions on  $Q$ .

But physics does not permit this enlargement of the gauge group. In physics, the scalar product  $(.,.)$  between two fast wave functions, which *a priori* is a function on  $SU(2)$ , must project down to a function on  $Q$  and thus be invariant under  $g \rightarrow gh$ . This is because scalar products are observable, and it is only functions on  $Q$  and not general functions on  $SU(2)$  which are observable. For it is  $Q$  and not  $SU(2)$  which is the configuration space.

Scalar products between any two  $\chi_m^F$ 's do not at all depend on  $g$ . We can assume that they are permissible fast wave functions. If  $\chi_{m'}^F \hat{v}_{m'n}(g)$  is also a permissible wave function, its scalar product with  $\chi_m^F$ ,

$$(\chi_m^F, \chi_{m'}^F \hat{v}_{m'n}(g)) = \hat{v}_{mn}(g), \quad (4.22)$$

must be a function on  $Q$ . So  $\hat{v}$  must be a  $\hat{u}$  with the property (4.21), and  $\mathcal{U}_{[\bar{\rho}]}$  is the gauge group.

## V. SYMMETRY RESTORATION: $\mathcal{P}, \mathcal{T}$ -DOUBLES AND HOW THEY SPLIT

### A. Symmetry Restoration

We have explained before that  $\mathcal{P}$  and  $\mathcal{T}$  get violated by a quantum shape having UIR  $\rho$  if  $\rho$  becomes an inequivalent UIR under their effect. For our  $Q$ , violation happens by  $\rho$  becoming its complex conjugate  $\bar{\rho} \neq \rho$ .

While quantum shapes can violate  $\mathcal{P}$  and  $\mathcal{T}$ , we cannot entertain the conjecture that a quantum molecule does so, its microscopic Hamiltonian being rigorously invariant under these symmetries. So  $\mathcal{P}$  and  $\mathcal{T}$ , even if spoilt by shapes, must become good again after the effect of the electronic cloud is accounted for. Let us once more explain this remarkable symmetry restoration.

When  $\rho$  becomes  $\bar{\rho}$  under  $\mathcal{P}$  or  $\mathcal{T}$ , the slow wave function  $\psi_S$  becomes  $\mathcal{K}\psi_S$  (where  $\mathcal{K}$  is either  $\mathcal{P}$  or  $\mathcal{T}$ ) and transforms by  $\bar{\rho}$ . If  $\rho \neq \bar{\rho}$ ,  $\mathcal{P}$  or  $\mathcal{T}$  does not leave the domain of the slow Hamiltonian invariant and spoils the symmetry. This is what we claimed in previous work [9].

We now include the electronic cloud. In discussing this cloud, it is necessary to clarify our assumption about the actions of  $\mathcal{P}$  or  $\mathcal{T}$  on the internal wave functions  $\alpha_j$  which are functions of  $\{\xi_\beta\}$ . Our assumption is that this action does not cause domain problems for the Hamiltonian. It is thus enough to pay attention to  $\rho$  and  $\bar{\rho}$ .

When  $\bar{\rho}$  changes to  $\rho$  under  $\mathcal{K}$ ,  $\chi^F$  becomes  $\mathcal{K}\chi^F$  and transforms by  $\rho$ . So while  $\psi_S^m \chi_m^F$  transforms by  $\rho \otimes \bar{\rho}$ . As for the complete wave function  $\phi = \psi_S^m \chi_m^F$ , it becomes

$$\mathcal{K}\phi = (\mathcal{K}\psi_S)^m (\mathcal{K}\chi^F)_m, \quad (5.1)$$

the first factor being associated with  $\bar{\rho}$  and the second with  $\rho$ . The overwhelming question is then whether  $\phi$  and  $\mathcal{K}\phi$  are in the domain of the full Hamiltonian  $\mathcal{H}$ .

Our hypothesis has been that the domain  $V^{(\rho_0)}$  of  $\mathcal{H}$  is associated with the untwisted bundle corresponding to the trivial UIR  $\rho_0$ . It thus consists of appropriately smooth functions on  $Q$ . Now  $\phi$  is invariant under the action of  $H^*$ ,

$$\phi(gh, \cdot) = \psi_S^{m'} \rho(h)_{m'm} \chi_{m''}^F \bar{\rho}_{m''m} \quad (5.2)$$

$$= \phi(g, \cdot) \quad (5.3)$$

and hence

$$\phi \in V^{(\rho_0)} \quad (5.4)$$

and is a function on  $Q$ . This is a relief: we would not be able to proceed further if  $\phi \notin V^{(\rho_0)}$ . A similar calculation shows that  $\mathcal{K}\phi$  too is  $H^*$ -invariant. We therefore have that

$$\mathcal{K}\phi \in V^{(\rho_0)}. \quad (5.5)$$

This shows that the quantum molecule preserves  $\mathcal{K} = \mathcal{P}$  or  $\mathcal{T}$  even though the quantum shape may spoil it.

But the effective Hamiltonian  $\hat{\mathcal{H}}_S$  does disturb  $\mathcal{K}$ -symmetry if  $\rho \neq \bar{\rho}$ . There is then no sense in applying  $\hat{\mathcal{H}}_S$  to  $\phi$  since the latter is not in the domain of  $\hat{\mathcal{H}}_S$  which is derived from the UIR  $\rho$ . *We thus see that an effective Hamiltonian can show spurious symmetry violations, which however get restored when fast degrees of freedom are judiciously included.* [8]. This could be a significant insight taught to us by the B-O approximation.

## B. Meaning of $\vec{L}_S$ in $\vec{\mathcal{L}}_S$

We now take up the precise definition of  $\vec{L}_S$  which occurs in (4.5). It is not the orbital angular momentum: orbital angular momentum acts on functions on  $Q$  whereas this  $\vec{L}_S$  acts on certain functions of  $g$  which for  $\rho \neq \bar{\rho}$  do not admit interpretation as suitably smooth functions on  $Q$ . We should use a different symbol for this  $\vec{L}_S$ , but we avoided that to prevent excessive early perplexity in the reader, if any.

We have shown that  $\phi$  is a function on  $Q$ . Hence  $\vec{L}_S$  is well-defined on  $\phi$  and acts as orbital angular momentum. Now the action  $g \rightarrow e^{i\vec{\theta} \cdot \vec{\tau}/2} g$  of  $SU(2)$  commutes with the action of  $H^*$ . So  $SU(2)$  acts on  $Q = SU(2)/H^* = \{gH^*\}$  and there becomes its rotations. It follows that if  $\vec{L}^{(\rho)}$  and  $\vec{L}^{(\bar{\rho})}$  are the generators of the above  $SU(2)$  acting on the argument  $g$  of  $\psi_S$  and  $\chi^F$ , then

$$\vec{L}_S \phi = [\vec{L}^{(\rho)} \psi_S^m] \chi_m^F + \psi_S^m [\vec{L}^{(\bar{\rho})} \chi_m^F]. \quad (5.6)$$

Hence

$$(\vec{\mathcal{L}}_S)_{mn} = \delta_{mn} \vec{L}^{(\rho)} + (\chi_m^F, [\vec{L}^{(\bar{\rho})} \chi_n^F]) \quad (5.7)$$

This then is the correct way to write  $\vec{\mathcal{L}}_S$ . We will henceforth follow the correct path and abandon the erroneous (4.5).



### C. On How Parity Doubles are Split

There is nothing here that cannot be inferred from [4]. But although not new, what follows is helpful to understand how the degeneracy of the doubles is lifted.

In the state  $\chi_m^F$ , the kets  $|m\rangle$  carry the UIR  $\bar{\rho}$  of  $H^*$ , while the group  $SU(2)$  acts on  $|k, j\rangle$  with generators  $\vec{L}_F$ . The total angular momentum is thus

$$\vec{J}_T = \vec{L}_F + \vec{L}_S. \quad (5.8)$$

The state  $\chi_m^F$  is a singlet under  $\vec{J}_T$  because

$$\begin{aligned} e^{i\vec{\theta} \cdot \vec{J}_T} \{|m', j\rangle D_{m'm}^j(g)\} &= \{U(e^{i\vec{\theta} \cdot \vec{\sigma}/2})|m', j\rangle\} \{D_{m'm}^j(e^{-i\vec{\theta} \cdot \vec{\sigma}/2}g)\} \\ &= |m', j\rangle D_{m'm}^j(g). \end{aligned} \quad (5.9)$$

Thus

$$\vec{J}_T \phi = (\vec{L}_S^{(\rho)} \otimes \mathbf{1}) \phi := [\vec{L}_S^{(\rho)} \psi_S^m] \chi_m^F. \quad (5.10)$$

With this result in mind, we write

$$\begin{aligned} \vec{L}_S &= \vec{L}_S^{(\rho)} \otimes \mathbf{1} + \mathbf{1} \otimes \vec{L}_S^{(\bar{\rho})} \\ &= \vec{L}_S^{(\rho)} \otimes \mathbf{1} + \mathbf{1} \otimes (\vec{J}_T - \vec{L}_F) \end{aligned} \quad (5.11)$$

and find

$$\vec{L}_S \phi = [\vec{J}_T \psi_S]^m \chi_m^F - \psi_S^m [\vec{L}_F \chi_m^F]_m. \quad (5.12)$$

In the leading B-O approximation,  $\vec{L}_F$  gets restricted to the span of  $\chi_m^F$  for  $m \in \bar{I}$  in the computation of  $\vec{L}_S$ . We will now see that our doubles are split by  $\mathcal{H}$  on removing this restriction.

The states  $\phi$  and  $\mathcal{K}\phi$  are not generally orthogonal. There is no reason for them to be so.

Let us first concentrate on  $\mathcal{K}$  being  $\mathcal{P}$  and form the orthogonal  $\mathcal{P} = \pm 1$  states, the superposition in its formation being permitted as both  $\phi$  and  $\mathcal{P}\phi \in V^{(\rho_0)}$ :

$$|\pm\rangle = \frac{\phi \pm \mathcal{P}\phi}{\sqrt{2}[1 \pm (\phi, \mathcal{P}\phi)]^{1/2}}, \quad (5.13)$$

$$\mathcal{P}|\pm\rangle = \pm|\pm\rangle. \quad (5.14)$$

Here we have used the hermiticity of  $\mathcal{P}$  and the attendant reality of  $(\phi, \mathcal{P}\phi)$ . For these states,

$$\begin{aligned} \mathcal{H}|\pm\rangle &= [\frac{1}{2\mathcal{I}}(\vec{J}_T^2 + \vec{L}_F^2) + \mathcal{H}_F]|\pm\rangle \\ &\quad - \frac{1}{\mathcal{I}\sqrt{2}[1 \pm (\phi, \mathcal{P}\phi)]^{1/2}} \{(\vec{J}_T \psi_S^m)(\vec{L}_F \chi_m^F) \pm (\vec{J}_T \mathcal{P}\psi_S^m)(\vec{L}_F \mathcal{P}\chi_m^F)\}. \end{aligned} \quad (5.15)$$

We can diagonalise  $\vec{J}_T^2$  along with  $\mathcal{H}$  so that the first term is proportional to  $|\pm\rangle$ . The ground state angular momenta for  $|\pm\rangle$  would also be equal. [The total angular momentum

and magnetic quantum number labels  $J$  and  $\sigma$  are for now suppressed.] So the first term does not split the energies of  $|\pm\rangle$ . As for the second term, as  $\vec{L}_F^2$  has value  $j(j+1)$  on  $|m, j\rangle$ , it serves to correct the equation determining  $\psi_j$ . It cannot help to split the parity doubles if  $\mathcal{H}_F$  fails to do so.

But the last term in (5.15) would generally split the doubles. Its scalar products with  $|\pm\rangle$ , which are the mean interaction energies from the perturbing Hamiltonian  $-\vec{J}_T \cdot \vec{L}_F / \mathcal{I}$ , are not the same for  $\mathcal{P} = \pm 1$  because of the differing normalization factors  $[1 \pm (\phi, \mathcal{P}\phi)]^{1/2}$  of (5.15).

In this manner, we see that the parity doubles are not degenerate in the exact theory.

#### D. Split $\mathcal{P}$ - Doubles are $\mathcal{T}$ - Doubles Too

We will assume in further work that the doubles  $|+\rangle$  and  $|-\rangle$  are certainly split. Now  $\mathcal{T}|\pm\rangle$  is degenerate with  $|\pm\rangle$  and hence by hypothesis cannot be  $|\mp\rangle$ . Therefore  $\mathcal{T}$  does not affect the eigenvalues of  $\mathcal{P}$  and  $\mathcal{P}$  and  $\mathcal{T}$  commute:

$$\mathcal{P}\mathcal{T} = +\mathcal{T}\mathcal{P}. \quad (5.16)$$

If  $\phi$  has total angular momentum  $J$  and its third component  $\sigma$ , we can write

$$\phi = |\sigma, J\rangle\chi \quad (5.17)$$

where  $|\sigma, J\rangle$  are orthonormal vectors transforming by the standard rotation matrices [18–20] and  $\chi$  are annihilated by  $\vec{J}_T$ . [We assume that there is no total angular momentum degeneracy for fixed energy for the states in question.] The unit norm of  $\phi$  fixes the norm of  $\chi$ .

It follows that the even and odd parity states can be taken to be

$$|\pm; \sigma, J\rangle = \frac{1}{\sqrt{2}[1 \pm (\phi, \mathcal{P}\phi)]^{1/2}}(\mathbf{1} \pm \mathcal{P})|\sigma, J\rangle\chi, \quad (5.18)$$

$$\mathcal{P}|\pm; \sigma, J\rangle = \pm|\pm; \sigma, J\rangle \quad (5.19)$$

where now the angular momentum labels of the states are also displayed.

The state  $\mathcal{T}|\epsilon; \sigma, J\rangle$  [ $\epsilon = \pm 1$ ] is linear in  $|\epsilon; J, \sigma\rangle$  by (5.16) and transforms under  $SU(2)$  according to

$$e^{i\vec{\theta} \cdot \vec{J}_T}(\mathcal{T}|\pm; \sigma, J\rangle) = (\mathcal{T}|\pm; \sigma', J\rangle)D_{\sigma'\sigma}^J(e^{i\vec{\theta} \cdot \vec{\sigma}/2})^* \quad (5.20)$$

because  $e^{i\vec{\theta} \cdot \vec{J}_T}$  commutes with  $\mathcal{T}$  and

$$e^{i\vec{\theta} \cdot \vec{J}_T}|\pm; \sigma, J\rangle = |\pm; \sigma', J\rangle D_{\sigma'\sigma}^J(e^{i\vec{\theta} \cdot \vec{\sigma}/2}). \quad (5.21)$$

It follows that

$$\mathcal{T}|\pm; \sigma, J\rangle = |\pm; \sigma', J\rangle C_{\sigma'\sigma} \quad (5.22)$$

where a possible phase on the right hand side has been set equal to 1 and  $C$  implements the equivalence between  $D^J$  and  $D^{J*}$ ,

$$C^{-1}D^JC = D^{J*}, \quad C^2 = (-1)^{2J}\mathbf{1}. \quad (5.23)$$

$C$  is the reduced rotation matrix for  $\pi$  rotation for the conventional phase choices of angular momentum matrices wherein the second angular momentum component is purely imaginary and the first and third components are real:

$$C = D^J[e^{i\pi\sigma_2/2}], \quad (5.24)$$

$$C_{\sigma'\sigma} = (-1)^{J-\sigma}\delta_{\sigma,-\sigma'}. \quad (5.25)$$

Note that

$$\mathcal{T}^2 = (\mathcal{PT})^2 = (-1)^{2J}. \quad (5.26)$$

Wigner has elsewhere shown [21] that we would have these identities if  $\mathcal{P}$  and  $\mathcal{T}$  are implemented on a space of states carrying a single UIR of spin cover of the rotation group.

### E. Split $\mathcal{T}$ -Doubles with the Same Parity

These occur for staggered conformations. Our assumption as before is that the doubles are certainly split. Given this hypothesis, we want to know the sort of linear combinations of states diagonalising  $\mathcal{H}$ .

Let us write

$$\begin{aligned} \phi &:= |\sigma, J\rangle_1 \chi, \\ |\sigma, J\rangle_1 &\equiv |\sigma, J\rangle \end{aligned} \quad (5.27)$$

and also let

$$\begin{aligned} \mathcal{T}\phi &= \mathcal{T}(|\sigma, J\rangle_1 \chi) \\ &= |\sigma', J\rangle_2 C_{\sigma'\sigma} \chi^*. \end{aligned} \quad (5.28)$$

Here  $|\sigma', J\rangle_2$  serves the role of  $|\sigma, J\rangle$  for  $\mathcal{T}\phi$  and  $C$  accounts for the fact that  $\mathcal{T}\phi$  transforms by  $D^{J*}$  under  $SU(2)$ . As in the case of  $\mathcal{P}$ , there is no reason for  $|\sigma, J\rangle_2 \chi^*$  to be orthogonal to  $|\sigma, J\rangle_1 \chi$ .

As for  $\mathcal{T}(\mathcal{T}\phi)$ , we can write [21]

$$\mathcal{T}^2\phi = \eta_T \phi, \quad \eta_T = +1 \text{ or } -1. \quad (5.29)$$

That being so, we have,

$$\mathcal{T}(|\sigma', J\rangle_2 \chi^*) = \eta_T |\sigma'', J\rangle_1 C_{\sigma''\sigma}^{-1} \chi, \quad (5.30)$$

since  $C^* = C$  under prevailing conventions [Cf (5.24) and (5.25)]. States of definite energy carry an irreducible representation of  $\vec{J}_T$  and so have a basis of vectors

$$z_1|\sigma, J\rangle_1 \chi + z_2|\sigma, J\rangle_2 \chi^*, z_i \in \mathbf{C}. \quad (5.31)$$

We want to determine  $z_i$  to the extent possible by general arguments. Let  $W$  be the vector space spanned by these states for fixed  $z_i$ . These states then have a fixed energy. If  $\mathcal{T}W \cap W = \{0\}$ , then  $W \oplus \mathcal{T}W$  will consist of all the  $\mathcal{T}$ -doubles, and they would be degenerate too since  $w \in W$  and  $\mathcal{T}w$  have the same energy. We have excluded this possibility by assumption. Now both  $W$  and  $\mathcal{T}W$  carry a UIR of  $SU(2)$  and so  $\mathcal{T}W \cap W$  is either  $W (= \mathcal{T}W)$  or  $\{0\}$ . Having already set aside the last possibility, we have

$$\mathcal{T}W = W. \quad (5.32)$$

Hence, remembering that  $\mathcal{T}$  reverses  $\sigma$  (and assuming that there is no angular momentum degeneracy for fixed energy for these states),

$$\mathcal{T}(z_1|\sigma, J\rangle_1 \chi + z_2|\sigma, J\rangle_2 \chi^*) = \omega_\sigma[z_1|-\sigma, J\rangle_1 \chi + z_2|-\sigma, J\rangle_2 \chi^*], \quad (5.33)$$

$$\mathcal{T}^2(z_1|\sigma, J\rangle_1 \chi + z_2|\sigma, J\rangle_2 \chi^*) = \omega_\sigma^* \omega_{-\sigma}(z_1|\sigma, J\rangle_1 \chi + z_2|\sigma, J\rangle_2 \chi^*) \quad (5.34)$$

where

$$|\omega_\sigma| = 1, \omega_\sigma \in \mathbf{C}. \quad (5.35)$$

But from (5.28), (5.29) and (5.30),

$$\mathcal{T}(z_1|\sigma, J\rangle_1 \chi + z_2|\sigma, J\rangle_2 \chi^*) = z_1^*|\sigma', J\rangle_2 C_{\sigma'\sigma} \chi^* + \eta_T z_2^*|\sigma', J\rangle_1 C_{\sigma'\sigma}^{-1} \chi, \quad (5.36)$$

$$\mathcal{T}^2(z_1|\sigma, J\rangle_1 \chi + z_2|\sigma, J\rangle_2 \chi^*) = \eta_T(z_1|\sigma, J\rangle_1 \chi + z_2|\sigma, J\rangle_2 \chi^*). \quad (5.37)$$

Comparing (5.33) and (5.34) with (5.36) and (5.37), we get

$$\omega_\sigma^* \omega_{-\sigma} = \eta_T, \quad (5.38)$$

$$z_1 \omega_\sigma = \eta_T z_2^* (-1)^{J+\sigma}, \quad (5.39)$$

$$z_2 \omega_\sigma = z_1^* (-1)^{J-\sigma}. \quad (5.40)$$

Either of the last two equations gives

$$|z_1| = |z_2| = \text{a constant } \lambda. \quad (5.41)$$

Hence,

$$z_i \neq 0. \quad (5.42)$$

Set

$$\omega_\sigma = (-1)^{J+\sigma} \omega. \quad (5.43)$$

Then,

$$|\omega_\sigma| = 1 \Rightarrow |\omega| = 1. \quad (5.44)$$

Now  $\omega$  is independent of  $\sigma$  by (5.39) since  $z_i \neq 0$ . Hence by (5.38), (5.39) and (5.40),

$$\eta_T = (-1)^{2J}, \quad (5.45)$$

$$z_1 \omega = \eta_T z_2^* \quad (5.46)$$

so that

$$z_i = \lambda e^{i\theta_i}, \quad (5.47)$$

$$\omega = \eta_T e^{-i(\theta_1 + \theta_2)}, \quad (5.48)$$

$$\theta_i = \text{real} \quad (5.49)$$

and

$$z_1 |\sigma, J\rangle_1 \chi + z_2 |\sigma, J\rangle_2 \chi^* = \lambda \{e^{i\theta_1} |\sigma, J\rangle_1 \chi + e^{i\theta_2} |\sigma, J\rangle_2 \chi^*\}. \quad (5.50)$$

In a particular model, states of a particular fixed energy will have a fixed value  $\tilde{\theta}_i$  for  $\theta_i$  and will be spanned by

$$e^{i\tilde{\theta}_1} |\sigma, J\rangle_1 \chi + e^{i\tilde{\theta}_2} |\sigma, J\rangle_2 \chi^*. \quad (5.51)$$

Their  $\omega$  will also be fixed to be some  $\tilde{\omega}$ :

$$\omega = \tilde{\omega} = \eta_T e^{-i(\tilde{\theta}_1 + \tilde{\theta}_2)}. \quad (5.52)$$

Another manifold of states with a fixed energy split from (5.51) will be spanned by vectors orthogonal to (5.51). These two sets of states span  $W \oplus \mathcal{T}W$ .

There remains the freedom in certain phase choices. Thus let

$$|\widetilde{\sigma, J}\rangle_i = e^{i\tilde{\theta}_i} |\sigma, J\rangle_i, \quad (5.53)$$

$$\tilde{\mathcal{T}} = e^{i(\tilde{\theta}_1 + \tilde{\theta}_2)} \mathcal{T}. \quad (5.54)$$

Then,

$$\tilde{\mathcal{T}} |\widetilde{\sigma, J}\rangle_1 = |\widetilde{\sigma', J}\rangle_2 C_{\sigma'\sigma}, \quad (5.55)$$

$$\tilde{\mathcal{T}} |\widetilde{\sigma, J}\rangle_2 = |\widetilde{\sigma', J}\rangle_1 C_{\sigma'\sigma}, \quad (5.56)$$

$$\tilde{\mathcal{T}}^2 = (-1)^{2J}, \quad (5.57)$$

and (5.51) takes the simple form

$$|\widetilde{\sigma, J}\rangle_1 \chi + |\widetilde{\sigma, J}\rangle_2 \chi^*. \quad (5.58)$$

## VI. $\mathcal{P}$ -, $\mathcal{T}$ - DOUBLES IN QUARK PHYSICS

There are several areas of particle physics with the potentiality to support  $\mathcal{K}$ -doubles. As always, it can be realized only when there are two well-separated time scales  $T_S$  and  $T_F$ ,

$$T_S/T_F \gg 1. \quad (6.1)$$

In addition, the expected life time  $\tau$  of a suspected double must be large compared to  $T_S$ :

$$\tau/T_S \gg 1 \quad (6.2)$$

If this inequality is violated, and a state decays before its slow core completes several revolutions, even unstable doubles are not likely to occur.

Let us now briefly examine typical multi-quark states which may support these doubles. Other areas of particle physics where the B-O approximation may work will be discussed in Section 8.

### A. Quark Physics

In a previous paper [8], we had examined three-quark systems, two of them forming the heavy core, and checked if there are favorable candidates compatible with (6.1) and (6.2). Our conclusion was that the spectra of  $cbu$  and  $cbd$  baryons are the best places to look for  $\mathcal{P}$ -,  $\mathcal{T}$ - doubles. The estimates for (6.1) and (6.2) were

$$T_S/T_F \sim 8.8 - 11, \quad (6.3)$$

$$\tau/T_S \sim 10^9. \quad (6.4)$$

We will argue below that these B-O states are not quark model states. They are also not covered by models using heavy quark symmetry (see [22] and references therein for a recent review of heavy quark symmetry) which typically have just one heavy quark.

In course of time, states with many quarks having properties like molecules would surely be found. Dibaryons such as the  $H$  with six quarks have already been predicted [23–26] and searched for [27–29]. Six-quark states for example, with a heavy core populated by  $c$ 's and  $b$ 's and a light cloud of  $u$ 's and  $d$ 's would be ideal for the successful application of the B-O approximation and hence also the search for  $\mathcal{P}$ -,  $\mathcal{T}$ - doubles. But the experimental formation of such states are obviously extremely hard for now.

Other possibilities of this sort would be states with both quarks and antiquarks. For example, we can look at  $(c\bar{b})(u\bar{d})$ . This is really the composite state of a heavy meson  $c\bar{b}$  with a light one  $u\bar{d}$  and the B-O approximation should work if  $c\bar{b}$  can be described by an arrow. But further study would be needed if a more complicated description along the lines of the chiral Lagrangian is called for.

### B. Born-Oppenheimer States Are Not Quark Model States

In the quark model for mesons and baryons, it is generally the case that the total orbital angular momentum of the quarks has a fixed value. We will now prove that the contrary is correct for the B-O wave function showing that these two models are different.

Let us write the fast wave function in the form (3.9). It has zero total angular momentum. So if  $\phi$  has total angular momentum  $J$  and magnetic quantum number  $\sigma$ ,  $\psi_S^m$  and  $\phi$  must have the forms

$$\psi_S^m(g) = c_J D_{\sigma m}^J(g), \quad m \in \bar{I}, \quad (6.5)$$

$$\phi(g, \cdot) = c_J \sum_{m,j} D_{\sigma m}^J(g) |k, j\rangle D_{km}^j(g) \alpha_j(\cdot) \quad (6.6)$$

where  $c_J$  is to be tuned to get 1 for the norm of  $\phi$  and where, as per (3.8), the index set  $\bar{I}$  is such that

$$D_{km}^j(gh) = \sum_{m' \in \bar{I}} D_{km'}^j(g) \bar{\rho}_{m'm}(h). \quad (6.7)$$

Orbital rotations are spatial rotations which do not affect spin and hence the kets  $|k, j\rangle$ . Therefore they are the  $SU(2)$  transformations on the left of  $g$ . Orbital angular momentum is then not sharp on the state (6.6), the latter being a superposition of states of orbital angular momenta from  $|J - j|$  to  $J + j$ . We thus see that the quark model and the B-O approximations are different.

### C. Signals For $\mathcal{P}$ -, $\mathcal{T}$ - Doubles

In molecular physics, there is a neat way of experimentally detecting parity doubles. It goes as follows [1].

Low energy excitations of molecules are rotational bands stacked on vibrational energies  $E_n$  (see for example, [30]). For a molecule with moment of inertia  $\mathcal{I}$ , they have energies  $E_n + J(J+1)/2\mathcal{I}$  with the angular momentum  $J$  assuming successive values. The separation  $E_{n'} - E_n$  of vibrational excitations is much larger than rotational energies. Now if the levels  $(n, J)$  for given  $n$  and  $J$  are non-degenerate (but for angular momentum degeneracy), then one of the transitions  $(n', J) \rightarrow (n, J)$  or  $(n', J \pm 1) \rightarrow (n, J)$  would be forbidden in the dipole approximation by parity conservation, and the corresponding spectral line would be weak. This is so because in this scenario, states of successive  $J$  and same  $n$  differ in parity. In this way, one can indirectly infer the existence of parity doubles.

As for  $\mathcal{T}$ - doubles with the same parity, we have not found any discussion of their experimental detection in chemistry. These doubles are similar to the ones that occur in the presence of Kramers' degeneracy (see for example, [31]). Their existence is usually inferred indirectly, from statistical properties, as in the case of diamagnetic susceptibility of certain rare earth elements.

In nuclear physics, there is no direct experimental detection of  $\mathcal{P}$ -doubles and there is no reported example of a  $\mathcal{T}$ - double of the same parity. Theory, involving rather elaborate calculations, predicts  $\mathcal{P}$ -doubles at certain energies, and when experiments find excitations with these energies, they are accepted as the predicted doubles [6,7].

We can think of no clean signals for the detection of  $\mathcal{P}$ - or  $\mathcal{T}$ - doubles in quark physics either. How is one to experimentally tell apart a B-O state from a quark model state? Lacking unambiguous means for this purpose, theory should be the ultimate judge in this matter for now.

## VII. TOWARDS A GENERAL B-O THEORY

In previous sections, we always thought of  $Q$  as  $SU(2)/H^*$  and assumed rotational invariance. While these assumptions are good for illustrative purposes, they are also limiting when  $Q$  is a general manifold and the system lacks an obvious and appropriate symmetry. Such being often the case in physics, it is progressive to work towards a general theory of the B-O approximation. That is what we will try here in this section. There are certainly many works of B-O approximation which are not dependent on symmetry. The novelty here is its emphasis on bundle theory and topology.

In the B-O approach, we are not concerned with the whole Hilbert space of the fast wave functions. That would be useless as any two infinite-dimensional (separable) Hilbert spaces are isomorphic. Rather we focus on the space of eigenstates  $\chi^F$  of the fast Hamiltonian  $\mathcal{H}_F$  for a fixed energy in the discrete spectrum. Often, this eigenspace corresponds to the set of ground states of  $\mathcal{H}_F$ . Being eigenstates of  $\mathcal{H}_F$ , they are also in the domain of  $\mathcal{H}_F$  and are thus associated with smooth sections of a vector bundle over the fast configuration space  $\{F\}$ . But this bundle structure is not central in the B-O approach and will not be mentioned henceforth.

That is not all: there is more to be said about fast dynamics. In the B-O approximation, we solve for  $\chi^F$  imagining that the slow variables are static. So  $\chi^F$  depends not just on  $\{F\}$ , but is sensitive also to  $q \in Q$  as a sort of background variable.

But there is no particular reason for  $\chi^F$  to be a suitably smooth function on  $Q$ . It is quite enough if the scalar product  $(\chi^F, \widetilde{\chi^F})$  of any two eigenstates of  $\mathcal{H}_F$  for the energy of interest is a smooth function on  $Q$ . The reason is that only probability densities are observable and wave functions are not.

But while  $\chi^F$ 's may not be smooth functions of  $Q$ , it turns out that they are multi-valued functions on  $Q$ . Their nature can be understood in the following manner modelled on the work of Shapere and Wilczek reproduced in [2].

Let us first fix a fiducial point  $q_0 \in Q$ . Assume that the slow system is initially at  $q_0$  and that we have a corresponding fast wave function  $\chi^F(q_0, \cdot)$ . Imagine now that the slow system is adiabatically dragged around in a loop  $\Gamma_{q_0}$  ending up again at  $q_0$ . That is, we slowly transport the slow system from  $q_0$  to  $q_0$  along this loop. All along this process, the fast wave function remains an eigenstate with energy varying continuously. Being in the point spectrum, there is no uncertainty about its value. [Level crossings are assumed not to occur]. So after the circuit  $\Gamma_{q_0}$ , energy returns to its original value. But what about  $\chi^F$ ?

$\chi^F$  need not return to its original value  $\chi^F(q_0, \cdot)$  but can undergo a unitary transformation. If  $N$  is the dimension of the eigenspace and  $\chi_m^F(q_0, \cdot)$  the components of  $\chi^F$  in some orthonormal basis for the eigenspace at  $q_0$ , then it could happen that

$$\chi_m^F(q_0, \cdot) \rightarrow \chi_{m'}^F(q_0, \cdot) u(\Gamma_{q_0})_{m'm}, \quad (7.1)$$

$u(\Gamma_{q_0})$  being an  $N \times N$  unitary matrix. This transformed wave function has the same eigenvalue as  $\chi_m^F(q_0, \cdot)$  and is normalized, so such a change in  $\chi_m^F(q_0, \cdot)$  can happen.

Let  $\Gamma_q$  be an unparameterized path from  $q_0$  to  $q$  so that only its geographical location in  $Q$  matters, and let  $\wp = \{\Gamma_q\}$  the path space of  $Q$  with base point  $q_0$  [32,10]. [The loop  $\Gamma_{q_0}$  above is a member of  $\wp$ .] It is clear now that  $\chi^F$  is not best thought of as a function on  $Q$ ,



but we can think of them as special sorts of functions on  $\wp$ . Writing  $\chi^F(\Gamma_q, \cdot)$  for the wave function  $\chi^F(q, \cdot)$  at  $q \in Q$ , their specialty comes from the property

$$\chi_m^F(\Gamma_{q_0} \cup \Gamma_q, \cdot) = \chi_{m'}^F(\Gamma_q, \cdot) u_{m'm}(\Gamma_{q_0}). \quad (7.2)$$

The curve  $\Gamma_{q_0} \cup \Gamma_q$  here is obtained by concatenation: one first travels  $\Gamma_{q_0}$  and then  $\Gamma_q$ .

The space  $\wp$  is a fibre bundle over  $Q$ . The projection map is

$$\pi : \wp \rightarrow Q \quad (7.3)$$

$$\Gamma_q \rightarrow q \quad (7.4)$$

and the fibre consists of all paths ending up at  $q$ .

The transformation law (7.2) is reminiscent of sections of vector bundles [33]. But  $\Gamma_{q_0}$ 's do not form a group when they are composed by concatenation of curves. We need to impose more structure on  $\Gamma_q$  to get a vector bundle out, and we shall soon do so.

As an eigenstate of  $\mathcal{H}_S$  or a wave function in its domain need not also be a function on  $Q$ , but can always be thought of as a function on  $\Gamma_q$  with an equivariance property like (7.2). That is enough to ensure that probability densities therefrom are functions on  $Q$ . We had previously made the trivializing assumption that equivariance was in fact invariance so that this wave function was a function on  $Q$ . Then as we saw, the slow wave function  $\psi_S$  has a transformation law (4.11) with  $u$  replaced by its complex conjugate  $u^*$  while the total wave function  $= (\psi_S^m \chi_m^F)$  is a function on  $Q$ .

When  $N > 1$ , there is a redundancy in aspects of the description wherein we allow both components of  $\chi^F$  and the argument  $\Gamma_q$  to vary for a fixed  $q$  [10]. But there is no need for us to be distracted by this issue: it is only of minor relevance to the present work, and does not damage the conclusions.

We shall now reproduce known examples of  $\chi^F$  by postulating particular dependences of  $u$  on  $\Gamma_{q_0}$ . They will turn  $u$ 's into representations of groups and thereby also lead us to the sought-for vector bundles.

### A. Flat Bundles

The nature of  $\chi^F$  here is governed by the fundamental group  $\pi_1(Q)$  of the manifold  $Q$  [10]. Let  $q_0$  be the base point for defining the homotopy groups and let us assume that  $u$  depends only on the homotopy class  $\langle \Gamma_{q_0} \rangle$  of the loop  $\Gamma_{q_0}$ . We can then write  $u(\Gamma_{q_0})$  as  $u(\langle \Gamma_{q_0} \rangle)$ . It is also easy to see that  $u$  defines a unitary representation of  $\pi_1(Q)$ . Let us assume it to be irreducible, the general case being a direct sum of UIR's. This case then corresponds to  $\chi^F$  being sections of associated bundles for a UIR of  $\pi_1(Q)$  [33], a result which can be briefly explained as follows.

Let  $\langle \Gamma_q \rangle$  be the equivalence class of paths homotopic to  $\Gamma_q$ . An element of the vector bundle for the representation  $u$  is an equivalence class

$$(\langle \Gamma_{q_0} \rangle, v), \quad v = (v^1, v^2, \dots, v^N), \quad (7.5)$$

the equivalence relation being

$$(\langle \Gamma_{q_0} \rangle, v) = (\langle \Gamma_{q_0} \cup \Gamma_q \rangle, vu(\langle \Gamma_{q_0} \rangle)). \quad (7.6)$$

The section defined by  $\chi^F$  is just

$$q \rightarrow (\langle \Gamma_q \rangle, \chi^F(\langle \Gamma_q \rangle, \cdot)). \quad (7.7)$$

So  $v$  above should be a function of  $\{F\}$  [just as  $\chi^F(\langle \Gamma_q \rangle, \cdot)$ ] to account for our case, but that is only a modest change.

In the same manner,  $\psi_S$  too can be regarded as a function of  $\langle \Gamma_q \rangle$  and defines a section of a vector bundle. Let us assume for illustration that  $\mathcal{H}_S$  acts on functions on  $Q$ . Once that is so, we can verify as before that differentials  $d$  on  $Q$  which would occur in  $\mathcal{H}_S$  become covariant differentials  $\nabla$  in the B-O approximation with the transformation

$$\nabla \rightarrow u[\langle \Gamma_q \rangle]^{-1} \nabla u[\langle \Gamma_{q_0} \rangle] \quad (7.8)$$

when  $\chi^F(\langle \Gamma_q \rangle, \cdot)$  is acted on by  $\pi_1(Q)$ :

$$\chi^F(\langle \Gamma_q \rangle, \cdot) \rightarrow \chi^F(\langle \Gamma_{q_0} \cup \Gamma_q \rangle, \cdot) \quad (7.9)$$

So if  $\mathcal{H}_S$  acts on functions on  $Q$ , the relevant UIR for  $\psi_S$  is  $u^*$ .

It remains to write the total wave function  $\phi$ . The best way to write it is probably

$$\phi(\langle \Gamma_q \rangle, \cdot) = \sum_{\langle \Gamma_{q_0} \rangle \in \pi_1(Q)} \psi_S^m(\langle \Gamma_{q_0} \cup \Gamma_q \rangle) \chi_m^F(\langle \Gamma_{q_0} \cup \Gamma_q \rangle, \cdot). \quad (7.10)$$

Being  $\pi_1(Q)$ -invariant, this  $\phi$  would give us a section of a trivial bundle over  $Q$  as we want.

The omission of the  $m$ -sum in (7.10) is intentional. Terms with different  $m$  are equal so that  $m$  can be frozen to any fixed value. We can prove this by writing (7.10) as

$$\sum_{\langle \Gamma_{q_0} \rangle \in \pi_1(Q)} \psi_{m'}^S(\langle \Gamma_q \rangle) u_{m'm}^*(\langle \Gamma_{q_0} \rangle) \chi_F^{m''}(\langle \Gamma_q \rangle) u_{m''m}(\langle \Gamma_{q_0} \rangle). \quad (7.11)$$

An easy application of orthogonality relations between  $u$ 's [34] gives

$$\sum_{\langle \Gamma_{q_0} \rangle \in \pi_1(Q)} u_{m'm}^*(\langle \Gamma_{q_0} \rangle) u_{m''m}(\langle \Gamma_{q_0} \rangle) = \delta_{m'm''}/N \quad (7.12)$$

which shows the result.

Elsewhere [32,10], we have explained that  $\{\langle \Gamma_q \rangle\}$  is just the universal cover  $\tilde{Q}$  of  $Q$ .

## B. $U(1)$ Bundles

Let us go step-by-step and see how to get  $U(1)$  bundles next. They are important for a wide variety of physical systems including the lowly  $N_2O$ .

The wave function  $\chi^F$  can always be thought of as a function on  $\wp$ . By the general argument above, we have the transformation law (7.2). If for a particular class of  $\Gamma_{q_0}$ , it happens that  $u(\Gamma_{q_0}) = 1$ , we can then identify  $\Gamma_q$  and  $\Gamma_{q_0} \cup \Gamma_q$  thereby getting a smaller space on which  $\chi^F$  is well-defined.

The universal cover  $\tilde{Q}$  is just one such space. In that case,  $u$  depends only on  $\langle \Gamma_q \rangle$ . Assuming that  $u$  is a faithful representation of  $\pi_1(Q)$ , we can then say that

$$\tilde{Q} = \wp / \sim. \quad (7.13)$$

where the equivalence relation is defined by

$$\Gamma_q \sim \Gamma'_q \Leftrightarrow u(\Gamma_q) = u(\Gamma'_q) \quad (7.14)$$

Occasionally, it is convenient to think of  $u(\Gamma_q)$  as the Wilson integral of a flat connection on  $\Gamma_q$  for this case:

$$u(\Gamma_q) = Pe^{\int_{\Gamma_q} A}, \quad A = \text{a flat connection} \quad (7.15)$$

The circumstance under which  $\chi^F$  becomes associated with a  $U(1)$  bundle is similar and has also been explained before [32]. There it is shown that the equivalence relation (7.14) turns  $\wp / \sim$  into a  $U(1)$  bundle if  $u$  has the form (7.15) where  $A$  is the connection of such a bundle.

Under our assumptions where  $\mathcal{H}_S$  acts on sections of a trivial bundle,  $\phi$  is associated with a trivial bundle as we have already seen.

### C. $G$ -Bundles

When  $u$  is characterized by a flat bundle, we get  $\tilde{Q}$ , and when it is given by a  $U(1)$ -connection, we get a  $U(1)$  bundle. In the same way, when  $u$  has the expression (7.15) where  $A$  is the connection for a  $G$ -bundle on  $Q$ ,  $\wp / \sim$  becomes the  $G$ -bundle as explained in [32,35]. In this case too, there is nothing further to add about the nature of  $\psi_S^m$  or  $\phi$ .

### D. Level Crossings

There is a serious deficiency in the above discussion. The same  $Q$  can often support twisted bundles and connections of different sorts, and we have not found any rule to tell which bundle and connection will occur when.

When  $H^*$  is discrete, so that  $Q = SU(2)/H^*$  has dimension three, there is a general theorem saying that all bundles on  $Q$  admit flat connections [36]. In other words, wave functions are sections of some associated  $\pi_1(Q)$  bundles [or rather of associated  $U_N$  bundles reducible to these flat bundles]. But we do not know exactly what the bundle and connection are without detailed knowledge of  $\chi^F$ . The UIR  $\bar{\rho}$  of  $H^*$  on the fast eigenspace does in fact fix the bundle, but it would be useful to know if the connection  $\nabla$  is flat or not.

For molecules,  $Q$  can be two-dimensional: it can be  $S^2$  or  $\mathbf{RP}^2$ . For the former, we can in fact tell the bundle and the connection with precision. If  $K$  is the eigenvalue of  $\vec{n} \cdot \vec{L}_F$ , the former is the  $U(1)$  bundle with Chern character  $K$ . Also, spatial rotations can be lifted to the bundle. The connection compatible with this lift is unique and is the well-known charge-monopole connection for the same  $K$ ,  $4\pi K$  being the product  $eg$  of electric and

magnetic charges  $e$  and  $g$  [10]. So for  $Q = S^2$ , we can tell the nature of the bundle by simple considerations.

Let us also check out  $\mathbf{RP}^2$ . The latter admits the flat  $\mathbf{Z}_2$  bundle  $S^2$  and an infinity of rank 2  $D_\infty$ -bundles as we saw in Section 2. We can tell what the bundle is once more from the UIR of  $H^*$ , but the properties of the connection remain vague without further input.

In one approach to the Berry phase [2], twisted bundles for fast variables arise from level crossings. In this point of view,  $Q$  can be embedded in a larger space  $\hat{Q}$ . Also there are points in  $\hat{Q}$  where two fast levels become degenerate, while they are not so in some neighbourhood of these points. In particular they do not cross on  $Q$ . The nature of the bundle on  $Q$  and its connection are then inferred using certain considerations developed by von Neumann and Wigner [37].

General discussions of this sort, at least for molecules, with good candidates for  $\hat{Q}$  would be worthwhile. We have not seen them in the literature.

## VIII. FINAL REMARKS

### A. Skyrmions and Monopoles

Parity and time-reversal doubles may well occur in Skyrmion and grand unified monopole physics [8]. For both Skyrmions and monopoles, there now exist elaborate simulations of static configurations for differing values of baryon number and monopole charge [38–42]. They are found as regular solids with discrete symmetry groups. We can imagine that further calculations will show static configurations such as a pear, with a  $U(1)$  symmetry group. Excitations with spin, like a  $\rho$  or an  $\omega$ , or even a nucleon, which can have non-zero helicity, can then lead to  $\mathcal{P}$ - and  $\mathcal{T}$ - doubles for Skyrmions. As for monopoles, by attaching fast constituents like a spin-half quark, we can hope to create these doubles in monopole physics too.

There is one potentially attractive application of the B-O method which is not directly tied up with  $\mathcal{P}$ ,  $\mathcal{T}$ - doubles. That is the following: In the original Skyrme approach [10,43–46], the soliton of the chiral model is interpreted as the nucleon. Spinorial quantization of the soliton is possible because the configuration space  $Q$  has double connectivity and the generator  $\pi_1(Q)$  in the baryon or winding number [43,44]  $\pm 1$  sector is got by rotating the soliton by  $2\pi$  [Cf [10] and references therein].

There is a second description of the nucleon which couples quarks as well to the chiral field. (See for example [47] and references therein). Controversies concerning double-counting has been generated by this approach.

But there is a possible reconciliation of these two models. Consider the chiral field coupled to three quarks and let us treat the former as slow and the latter as fast. Assume furthermore that the slow Hamiltonian  $\mathcal{H}_S$  for the winding number 1 or -1 is to be quantized with tensorial states. Our general considerations show that the effective Hamiltonian  $\hat{\mathcal{H}}_S$  after integrating out quarks acts on spinorial states. Thus  $\hat{\mathcal{H}}_S$  is the Hamiltonian in the Skyrme approach whereas  $\mathcal{H}_S + \mathcal{H}_F$  is the Hamiltonian close to the model with explicit quark fields.

There are details to be attended to before we can be confident of this reconciliation. Work on these matters is in progress.

## B. Heavy Meson Bound States

Baryons, chiral solitons and monopoles are not the only favorable systems for the application of the B-O ideas, even in particle physics. Literature abounds in speculation suggesting the existence of heavy meson bound states which can involve distinct mesons too [48,49]. They can be the slow variables and suitable excitations the fast ones and B-O approximation may be applicable. There may even be  $\mathcal{P}, \mathcal{T}$  doubles among these mesons.

## C. Anomalies

The derivation of anomalies using the adiabatic approximation is well understood in field theory [50–55]. Typically, in this approach to anomalies, gauge fields are regarded as classical background fields and anomalies are deduced from the response of the fermion determinant or of its Fock vacuum to gauge transformations. We must think of gauge fields as slow variables in this method and the spinorial fields as fast.

We found a similar situation when studying  $\mathcal{P}, \mathcal{T}$ -doubles. When there are  $\mathcal{P}$ -doubles for example, the ground state (say) of  $\mathcal{H}_F$  is not  $\mathcal{P}$ -invariant just as the Fock vacuum is not gauge invariant if there are gauge anomalies [53]. There is also no sense in superposing the ground state  $\chi^F$  and its  $\mathcal{P}$ -transform  $\mathcal{P}\chi^F$  and enforcing  $\mathcal{P}$  invariance (or  $\mathcal{P} = -1$ ), as the scalar product  $(\chi^F, \mathcal{P}\chi^F)$  and the probability densities of these superpositions are not functions on  $Q$ . We cannot thus impose the condition  $\mathcal{P} = 1$  on a fast state, just as we cannot impose gauge invariance on Fock vacuum if there is a gauge anomaly.

But the situation changes for parity on including slow variables. The derivatives in the slow Hamiltonian become covariant derivatives after averaging over  $\chi^F$ . This twists the slow bundle inducing a  $\mathcal{P}$ -anomaly there as well in such a way that there is no  $\mathcal{P}$ -anomaly in the total slow times fast wave functions. We can form total wave functions with  $\mathcal{P} = \pm 1$  and if appropriate retain only the  $\mathcal{P} = +1$  state.

It is natural to enquire if similar circumstances prevail in anomalous gauge theories. If that were so, the anomaly in the gauge response of the Fock vacuum would be cancelled by another anomalous response from the gauge field wave function, and there would be no anomaly left in the total state of the gauge and Fermi fields. [We remark here that Federbush [55] has found a regularisation of two-dimensional chiral gauge theories with no axial anomalies. See also [54] and references therein.]

There are indications that this is exactly what happens. When the Fock vacuum as constructed by Segal [53] is averaged out, the derivative  $\delta/\delta A_i$  in the Yang-Mills part acquires a connection showing the anomalous gauge response of the gauge field state. Just as for molecules, it can cancel the Fock space anomaly. The calculations showing these results are very similar to those in molecular physics.

It seems that the effect of the connection in the slow system can be accounted for by a gauged Wess-Zumino action in the Yang-Mills Lagrangian. This modified Lagrangian  $\hat{L}_S$  must be the Lagrangian leading to the Hamiltonian  $\hat{\mathcal{H}}_F$ .

A solution of this kind to the anomaly problem has been proposed before by Faddeev [52]. We suggest that it can be justified in the B-O approach as outlined above.

These remarks on anomalies are only in the nature of a report on work in progress. We hope to give a detailed account soon.

### D. Quantum Gravity

If  $M_1$  and  $M_2$  are two  $N$ -manifolds, their connected sum  $M_1 \# M_2$  is a new  $N$ -manifold. It is obtained by first removing  $N$ -balls  $B_N^{(i)}$  from  $M_i$  and then identifying the boundary spheres of  $M_i \setminus B_N^{(i)}$ . [For more details, see for example [10].]

In two and three dimensions, there exist the so-called prime manifolds  $P_i$  [10]. Any asymptotically flat two- or three-manifold with one asymptotic region is the connected sum of  $R^2$  or  $R^3$  and finitely many primes. The two-dimensional primes are  $T^2$  and  $RP^2$ , while there are infinitely many primes in dimension three.

Some time ago, Friedman and Sorkin [56,57] suggested the possibility of spatial slices in gravity theories with primes attached and argued that a prime is to be associated with an elementary excitation, a quantum “geon”. Friedman, Sorkin [56,57], Witt [58,59] and Surya [60] have established that  $\pi_1(Q)$  of the configuration space  $Q$  in the presence of primes is complicated, and implies, just as for Skyrmons or molecules, that quantization for gravity is not unique. Quantum gravity with spinorial geons may exist even for Einstein Lagrangian with no matter fields [56,57]. Quantum geons violating the familiar spin-statistics connection can also be found [61,33] in canonical gravity.

We would like to suggest that even in conservative gravity which ignores these quantization ambiguities and sticks to the trivial UIR of  $\pi_1(Q)$ , many other UIR’s can turn up in the presence of fast degrees of freedom. Thus for example a spinorial constituent attached to a tensorial geon can, after integrating out the fast variables, lead to an effective geon Hamiltonian  $\hat{\mathcal{H}}_S$  for a spinorial geon. In this way, we may induce many UIR’s of  $\pi_1(Q)$ . We are currently looking at this possibility. If correct, it would mean that non-trivial UIR’s of  $\pi_1(Q)$  cannot be ignored even in conservative gravity.

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